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**Microbial co-existence and stable equilibria  
in a mechanistic model of enteric methane  
production**

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Yuancheng Wang

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# Abstract

Globally, 14.5% of all anthropogenic greenhouse gases come from ruminants. One of these is methane, which is produced in the rumen of ruminant animals. Feed is degraded by microbes to produce volatile fatty acids (which are absorbed by the animal) and hydrogen (which is metabolized by methanogens to form methane). The dynamics of hydrogen production and metabolism are subject to thermodynamic control imposed by the hydrogen concentration. Existing models to estimate methane production are based on calculation of hydrogen balances without considering the presence of methanogens and do not include thermodynamic control. In this project, a model is developed based on glucose-hydrogen-methanogen dynamics to estimate methane production and illustrates a co-existence of microbes that employs different fermentation pathways competing for the same food source in the rumen. Glucose was chosen as an example of a fermentable feed component. A thermodynamic term was integrated into a Monod-type model to represent the thermodynamic control of hydrogen concentration on the rates of hydrogen generation and hydrogen metabolism. Results of this model suggest that the microbial community composition and the combination of the different pathways are determined by the rumen environment, biological parameters of the microbes and the feedback imposed by substrate and product concentrations. The mathematical enunciation of this model is therefore consistent with biological expectations. This model could be expanded to include plant polymer degradation rate, feeding level and feeding frequency to explore their effects on methane production. This model could also be integrated into models of whole rumen function to address more complex questions. It would also support experimentation

with animals for understanding factors that control methane formation and to explore methane mitigation strategies.

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# Abbreviations

|                  |   |
|------------------|---|
| ADP              | Adenosine diphosphate   |
| ATP              | Adenosine triphosphate<br>(used by microbes for maintenance and reproduction) |
| VFA              | Volatile fatty acids (e.g., acetate, propionate and butyrate)                 |
| HM               | Hydrogen-methanogen dynamics  |
| HM <sup>θ</sup>  | Hydrogen-methanogen dynamics with thermodynamic term                          |
| GHM <sup>θ</sup> | Glucose-hydrogen-methanogen dynamics with thermodynamic term                  |



# Nomenclature

## Subscript

| Substrate | Description |
|-----------|-------------|
| $h$       | hydrogen    |
| $g$       | glucose     |
| $A$       | acetate     |
| $P$       | propionate  |
| $B$       | butyrate    |

| Microbe | Description        |
|---------|--------------------|
| $m$     | methanogens        |
| $i$     | glucose fermenters |

## Superscript

| Notation | Description  |
|----------|--|
| $*$      | equilibrium point (steady state solution) of variables |

## Variables

| Notation | Description                  | Unit                                |
|----------|------------------------------|-------------------------------------|
| $t$      | time                         | s                                   |
| $S$      | substrate concentration      | mol ml <sup>-1</sup>                |
| $X$      | microbe population density   | cell ml <sup>-1</sup>               |
| $\theta$ | thermodynamic term           | unitless                            |
| $M$      | estimated methane production | rumen <sup>-1</sup> d <sup>-1</sup> |

## Parameters

| Rumen environment | Description                    | Unit                                 |
|-------------------|--------------------------------|--------------------------------------|
| $\alpha$          | passage rate through the rumen | s <sup>-1</sup>                      |
| $\beta$           | rate of substrate generation   | mol ml <sup>-1</sup> s <sup>-1</sup> |
| $\gamma$          | absorption rate of substrate   | s <sup>-1</sup>                      |

| Microbe | Description   | Unit  |
|---------|---|---|
| $q$     | maximal rate at which a microbe can metabolize substrate                  | mol cell <sup>-1</sup> s <sup>-1</sup>                |
| $K$     | substrate concentration at half of $q$ assuming no thermodynamic feedback | mol ml <sup>-1</sup>                                  |
| $w$     | moles of product generated from metabolizing per mole of substrate        | unitless  |
| $n$     | ATP gained by microbe from metabolizing per mole of substrate             | mol <sub>ATP</sub> mol <sup>-1</sup>                  |
| $m$     | maintenance requirement of a microbe                                      | mol <sub>ATP</sub> cell <sup>-1</sup> s <sup>-1</sup> |
| $Y$     | reproduction coefficient of microbe                                       | cell mol <sub>ATP</sub> <sup>-1</sup>                 |
| $\mu$   | reproduction rate of microbe  | s <sup>-1</sup>                                       |
| $d$     | death coefficient of microbe  | s <sup>-1</sup>                                       |

| Thermodynamic term | Description   | Unit                                 |
|--------------------|---|--------------------------------------|
| $T$                | temperature   | K                                    |
| $\mathcal{R}$      | ideal gas constant  | kJ mol <sup>-1</sup> K <sup>-1</sup> |
| $\Delta G_T^o$     | Gibbs free energy of a chemical reaction at $T$ under standard conditions | kJ mol <sup>-1</sup>                 |
| $\Delta G_{ATP}$   | energy required to generate one unit of ATP                               | kJ mol <sub>ATP</sub> <sup>-1</sup>  |